

vasicinone

Inchi: InChI=1S/C11H12N2O2/c14-9-5-6-13-10(9)12-8-4-2-1-3-7(8)11(13)15/h1-4,9,11,14-15H,1-2,7,10,12,13,15H2
InchiKey: AKRGPMZFCFDFQW-UHFFFAOYSA-N
Formula: C11H12N2O2
SMILES: OC1CCN2C1=Nc1cccc1C2O
Mol. weight [g/mol]: 204.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Aqueous Solubility Prediction Method
logp	0.788		Crippen Method
mcvol	147.770	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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